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Low-density cellular materials with optimal conductivity and bulk modulus

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Abstract :

Optimal upper bounds on the average conductivity and the bulk modulus of low density cellular materials are established. These bounds are tighter than the classical Hashin-Shtrikman upper bounds, and can be applied to anisotropic materials. Furthermore, necessary and sufficient conditions on the microgeometry of the cellular materials to maximize (for a given solid volume fraction) either the average conductivity or the bulk modulus are derived. The conditions are found to be identical for both quantities, so that the bounds are attained simultaneously: a low-density cellular material with maximal average conductivity will have maximal bulk modulus as well.

Résumé :

Des bornes optimales sur la conductivité moyenne et le module de compression de matériaux cellulaires de faible densité sont établies. Ces bornes sont plus précises que les bornes de Hashin-Shtrikman, et sont même applicables à des matériaux anisotropes. De plus, on établit des conditions nécessaires et suffisantes sur la structure des matériaux cellulaires afin que leur conductivité moyenne ou leur module de compression soit maximal(e). En fait, ces conditions se trouvent être les mêmes pour ces deux grandeurs, si bien que les bornes sont atteintes simultanément. Ainsi, un matériau cellulaire ayant une conductivité moyenne maximale aura également un module de compression maximal.

Key-words :

optimization ; conductivity ; bulk modulus

1 Introduction

Cellular materials appear widely in nature and are manufactured on a large scale by man. Examples include wood, cancellous bone, cork, or foams for insulation and packaging. Obviously, the transport and mechanical properties of such materials depend on the material density ϕ , defined as the volume of the continuous phase per unit volume of the material. However, for a given value of ϕ , these properties depend also on the specific distribution of the continuous phase. Various theoretical studies on the transport and mechanical properties of both two-dimensional (2D) and three-dimensional (3D) structures have been attempted. Unfortunately, exact calculations can be achieved for cellular materials with simple geometry only, and numerical simulations or semi-empirical models are required in order to study the properties of more complex structures. Nevertheless, expression of bounds on the effective electrical (or thermal) conductivity and elastic moduli can be established. Perhaps the most famous bounds are those given by Z. Hashin and S. Shtrikman for isotropic heterogeneous media [Hashin (1965); Hashin-Shtrikman (1962, 1963)]. When the transport and mechanical properties of the discontinuous phase are equal to zero, and in the low-density asymptotic limit ($\phi \ll 1$), the Hashin-Shtrikman (HS) bounds for the effective conductivity σ and the effective bulk modulus κ read as:

$$0 \leq \sigma^{(2D)} \leq \frac{\sigma_0 \phi}{2} \quad (1) \quad 0 \leq \kappa^{(2D)} \leq \frac{E_0 \phi}{4} \quad (2)$$

$$0 \leq \sigma^{(3D)} \leq \frac{\sigma_0 \phi}{3} \quad (3) \quad 0 \leq \kappa^{(3D)} \leq \frac{4E_0 \phi}{9} \frac{G_0 + 3K_0}{4G_0 + 3K_0}, \quad (4)$$

respectively for 2D [Hashin (1965); Torquato *et al.* (1998)] and 3D [Hashin-Shtrikman (1962, 1963)] structures. σ_0, E_0, G_0, K_0 are the conductivity, Young modulus, shear modulus, and bulk modulus of the continuous phase, respectively. The three elastic moduli E_0, G_0 , and K_0 are related by $E_0 = \frac{4K_0 G_0}{K_0 + G_0}$ for 2D bodies, and $E_0 = \frac{9K_0 G_0}{3K_0 + G_0}$ for 3D bodies.

The question we raise in the present study is whether there can be an optimal way to distribute the continuous phase in order to maximize the average conductivity or the bulk modulus of a low-density cellular material. In a recent study, Torquato *et al.* [Torquato *et al.* (1998); Hyun-Torquato (2002)] identified values of conductivity and elastic moduli of the two-dimensional square, hexagonal, kagomé and triangular cellular structures, and observed that the conductivity and the bulk modulus of these structures are equal to the respective HS upper-bound values. Indeed, we show in the present study that the two quantities always attain their respective bounds simultaneously. In the first part of the paper, we present an alternative and extended derivation of the HS bounds for the average conductivity of anisotropic structures, and show that the following criteria constitute a set of necessary and sufficient conditions to maximize the average conductivity (for a given value of ϕ):

- a) All the edges are straight.
- b) Each edge (i, j) has a uniform cross-section area s_{ij} .
- c) Every junction (i) between edges satisfies $\sum_j s_{ij} \mathbf{e}_{ij} = \mathbf{0}$, where \mathbf{e}_{ij} are outward-pointing unit vectors in the directions of adjoining edges.

In the second part, we derive bounds for the bulk modulus of cellular materials, which are identical or tighter than the HS bounds, and show the bulk modulus attains its maximal value under the very same necessary and sufficient conditions a), b), c).

2 Maximal average conductivity

Definition. On a macroscopic scale, a cellular material can be seen as a continuous medium, *a priori* anisotropic, whose transport properties are described by a symmetrical conductivity tensor $[\sigma]$ such that the electric field \mathbf{E} and the current density vector \mathbf{j} are related by: $\mathbf{j} = [\sigma] \cdot \mathbf{E}$. The density of dissipative energy per unit time is defined as: $P^* = \mathbf{j} \cdot \mathbf{E} = |\mathbf{E}|^2 \mathbf{n} \cdot [\sigma] \cdot \mathbf{n}$, where \mathbf{n} is the unit vector along the electric field. We define the *average conductivity* $\langle \sigma \rangle$ of a medium as the constant of proportionality between the averaged dissipated energy per unit volume and unit time $\langle P^* \rangle$ and the square of the external electric field modulus $|\mathbf{E}|^2$ when averaged on all the directions of the electric field: $\langle \sigma \rangle = |\mathbf{E}|^2 / \langle P^* \rangle = \langle \mathbf{n} \cdot [\sigma] \cdot \mathbf{n} \rangle$. It can be shown [Durand *et al.* (2004); Durand-Weaire (2004)] that $\langle \sigma \rangle$ is related to the trace of the conductivity tensor as $\langle \sigma \rangle^{2D} = \frac{1}{2} \text{Tr}([\sigma])$ for a 2D material, and $\langle \sigma \rangle^{3D} = \frac{1}{3} \text{Tr}([\sigma])$ for a 3D material.

Upper bound. The expression of an upper bound on $\langle \sigma \rangle$ can be easily established using Dirichlet's Principle (also known as dual form of Thomson's Principle). Consider a domain \mathcal{D} of a material with conductivity σ_0 . Dirichlet's Principle (which happens to be a theorem) states that *among all the twice continuously differentiable potential fields $V(\mathbf{r})$ satisfying the same boundary condition $V(\mathbf{r}) = f(\mathbf{r})$ on the boundary of \mathcal{D} , the potential function which satisfies Laplace equation $\nabla^2 V = 0$ is the one that makes the dissipated power $P = \sigma_0 \int_{\mathcal{D}} |\nabla V|^2 d\mathbf{r}$ an*

absolute minimum. In other words, the actual potential function V^* (the one satisfying Ohm's law $\mathbf{j} = -\sigma_0 \nabla V^*$ and steady condition $\nabla \cdot \mathbf{j} = 0$) is the one that minimizes P .

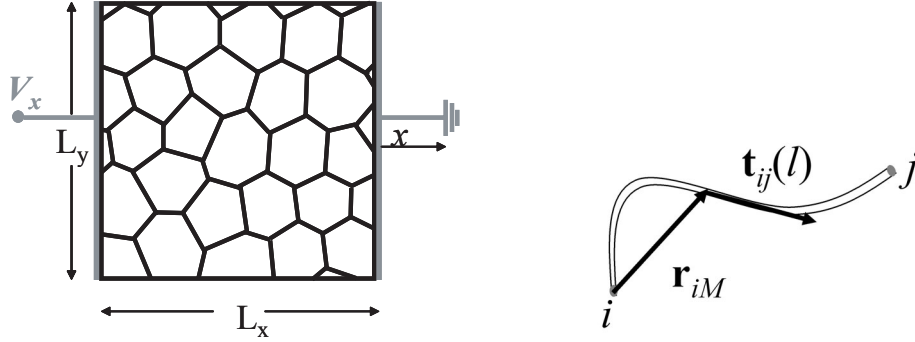


Figure 1: **a.:** Rectangular portion of a 2D cellular network subjected to a uniform difference of potential V_x between the two opposite faces $x = 0$ and $x = L_x$. We define the effective conductivity of the material in the x direction as $\sigma_x = \frac{L_x}{L_y} \frac{I_x}{V_x}$, where I_x is the total current through the network. **b.:** Schematic of a particular edge (i, j) . l denotes the curvilinear coordinate of a given point M along the edge. \mathbf{r}_M and \mathbf{t}_{ij} are respectively the position vector of point M taken from node i and the local tangent unit vector.

Imagine first a 2D cellular material made of edges, which *a priori* can be curved and with non-uniform cross-sections. In the low-density limit, the edges are very thin, so we can unequivocally define for each edge (i, j) a length l_{ij} , and a local cross-sectional area $s_{ij}(l)$ which varies with the curvilinear coordinate l along the edge (see Fig. 1b). Suppose that a macroscopic rectangular sample of that cellular material is placed between two parallel plates perpendicular to the x direction, as depicted on Fig. 1a. The plate $x = 0$ is brought to potential value V_x and the plate $x = L_x$ is connected to the ground. P^* , the minimal value of P , is given by: $P^* = V_x I_x$, where I_x is the total flow rate through the sample. For thin edges, the dissipated power can be rewritten $P = \sum_{(i,j)} (V(\mathbf{r}_i) - V(\mathbf{r}_j))^2 / R_{ij}$, where $R_{ij} = \frac{1}{\sigma_0} \int_0^{l_{ij}} \frac{dl}{s_{ij}(l)}$ is the resistance of edge (i, j) . The potential function defined as:

$$V = V_x (1 - x/L_x) \quad (5)$$

is twice continuously differentiable and satisfies the boundary condition. Using Dirichlet's principle with this trial potential function, we obtain: $P^* \leq \left(\frac{V_x}{L_x}\right)^2 \sum_{(i,j)} (x_j - x_i)^2 / R_{ij}$. The diagonal element σ_x , defined by: $V_x = \frac{L_x}{\sigma_x L_y} I_x$ is then bounded as:

$$\sigma_x \leq \frac{1}{L_y^2} \sum_{(i,j)} \frac{(x_j - x_i)^2}{R_{ij}}. \quad (6)$$

Let us now apply a potential difference V_y between two infinite plates perpendicular to the y direction. Using the same argumentation as before with the trial potential function:

$$V = V_y (1 - y/L_y) \quad (7)$$

(L_y is the distance between the two plates), it comes that σ_y is bounded as:

$$\sigma_y \leq \frac{1}{L_x^2} \sum_{(i,j)} \frac{(y_j - y_i)^2}{R_{ij}}. \quad (8)$$

Using the inequality ($s_{ij}(l)$ being always positive):

$$\int_0^{l_{ij}} \frac{dl}{s_{ij}(l)} \geq l_{ij}^2 / \int_0^{l_{ij}} s_{ij}(l) dl, \quad (9)$$

and introducing $\phi = \sum_{(i,j)} \int_0^{l_{ij}} s_{ij}(l) dl / (L_x L_y)$, it comes that $R_{ij} \geq l_{ij}^2 / (\sigma_0 \phi L_x L_y)$. Using this

bound on R_{ij} , we obtain: $\sigma_x \leq \sigma_0 \phi \sum_{(i,j)} \frac{(x_j - x_i)^2}{l_{ij}^2}$ and $\sigma_y \leq \sigma_0 \phi \sum_{(i,j)} \frac{(y_j - y_i)^2}{l_{ij}^2}$. Moreover, since:

$$(x_j - x_i)^2 + (y_j - y_i)^2 \leq l_{ij}^2, \quad (10)$$

we finally get:

$$\langle \sigma \rangle^{2D} \leq \frac{\sigma_0 \phi}{2}. \quad (11)$$

The argumentation is transposable with no difficulty to 3D materials: in that case, the average conductivity is bounded as:

$$\langle \sigma \rangle^{(3D)} \leq \frac{\sigma_0 \phi}{3}. \quad (12)$$

Note that the bounds 11 and 12 are identical to the HS bounds 1 and 3.

Criteria for maximal average conductivity. Let us now show that the three conditions a), b), c) are necessary and sufficient to maximize $\langle \sigma \rangle^{2D}$. Indeed, $\langle \sigma \rangle^{2D}$ attains its maximal value *if and only if* inequalities 6, 8, 9, and 10 are strict equalities. According to Dirichlet's principle, inequalities 6 and 8 become strict equalities when the respective trial potential functions 5 and 7 are the actual potential functions. In particular, the current distributions deriving from these potential functions must satisfy the equation of conservation along each edge and at each junction. Let us note $\mathbf{t}_{ij}(l)$ the local tangent unit vector along the edge (i, j) , I_{ij}^x the current in (i, j) associated with the potential function 5, and I_{ij}^y the current associated with the potential function 7. Both $I_{ij}^x = \sigma_0 s_{ij}(l) \mathbf{t}_{ij}(l) \cdot \mathbf{e}_x = \sigma_0 s_{ij}(l) \cos \alpha_{ij}(l)$ and $I_{ij}^y = \sigma_0 s_{ij}(l) \mathbf{t}_{ij}(l) \cdot \mathbf{e}_y = \sigma_0 s_{ij}(l) \sin \alpha_{ij}(l)$ must be independent of the curvilinear coordinate l . Obviously, the only way this can be satisfied is that the edge (i, j) is straight and has a uniform cross section. Under these conditions, which are nothing else but conditions a) and b), the two inequalities 9 and 10 become strict equalities as well. Finally, the equation of conservation at each junction (i) with the respective flow rates $I_{ij}^x = \sigma_0 s_{ij} \mathbf{e}_{ij} \cdot \mathbf{e}_x$ and $I_{ij}^y = \sigma_0 s_{ij} \mathbf{e}_{ij} \cdot \mathbf{e}_y$ gives $\mathbf{e}_x \cdot \sum_j s_{ij} \mathbf{e}_{ij} = 0$ and $\mathbf{e}_y \cdot \sum_j s_{ij} \mathbf{e}_{ij} = 0$. These two scalar equalities are indeed equivalent to condition c) for 2D networks. Once again, generalization to 3D materials is straightforward.

3 Maximal bulk modulus

Definition. Consider a circular portion of a 2D material, of radius R , and suppose that a uniform radial displacement $-\delta R \mathbf{e}_r$ is imposed on its boundary (\mathbf{e}_r is the radially oriented unit vector; the body is under uniform tension when $\delta R < 0$, and under uniform compression when $\delta R > 0$). We define the 2D bulk modulus $\kappa^{(2D)}$ of this structure as: $\kappa^{(2D)} = \pi R^2 \delta P / (2\pi R \delta R) = R \delta P / (2\delta R)$, where δP is the average load applied on the boundary. Similarly, we define the bulk modulus $\kappa^{(3D)}$ associated with a spherical portion of material of radius R as: $\kappa^{(3D)} = \frac{4}{3} \pi R^3 \delta P / (4\pi R^2 \delta R) = R \delta P / (3\delta R)$. We must point out that this definition is different from the one usually given for the bulk modulus: in the present definition, a uniform *displacement*,

rather than a uniform radial *load*, is imposed on the surface of the material. This definition allows to extend the notion of bulk-modulus to non-isotropic materials, and the two definitions are of course equivalent for isotropic materials.

Upper bound. The expression of an upper bound can easily be established using the principle of minimum potential energy. Let us note C_{ijkl} the components of the elastic tensor, and $u_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right)$ the components of the strain tensor associated with the displacement field $\mathbf{u}(\mathbf{r})$. The principle of minimum potential energy states that, *among all kinematically admissible displacement fields (i.e. any displacement field twice continuously differentiable satisfying the displacement constraints on the boundary), the actual displacement (i.e. the one satisfying the equations of mechanical equilibrium) is the one that makes the potential energy $U = \frac{1}{2} \int_{\mathcal{D}} \sum_{ijkl} C_{ijkl} u_{ij} u_{kl} d\mathbf{r}$ an absolute minimum.* Let us choose as kinematically admissible displacement field: $\mathbf{u}(\mathbf{r}) = -\frac{\delta R}{R} \mathbf{r}$, and let us evaluate the potential energy associated with. We assume the cross-section of each edge is sufficiently small so $\mathbf{u}(\mathbf{r})$ is uniform on it (or equivalently, we suppose $\mathbf{u}(\mathbf{r})$ is a macroscopic field which has a uniform value on the edge cross-section). Consider an infinitesimal piece of a given edge (i, j) , of length dl and cross-sectional area $s_{ij}(l)$. We denote \mathbf{r}_M and $\mathbf{r}_M + d\mathbf{r}$ the position of its two ends. Their relative displacement $(\mathbf{u}(\mathbf{r}_M + d\mathbf{r}) - \mathbf{u}(\mathbf{r}_M))$ is colinear to the local tangent unit vector $\mathbf{t}_{ij} = \frac{d\mathbf{r}}{dl}$, meaning that the piece of edge deforms by axial compression only. The force $\mathbf{F}_{ij}(l)$ acting on the surface $s_{ij}(l)$ is parallel to \mathbf{t}_{ij} and given by: $\mathbf{F}_{ij}(l) = E_0 s_{ij}(l) \frac{\delta R}{R} \mathbf{t}_{ij}$, where E_0 is the Young modulus of the solid phase. The strain energy associated with such a deformation is $\frac{E_0}{2} s_{ij}(l) \left(\frac{\delta R}{R} \right)^2$. Invoking addi-

tivity of the potential energy, and introducing the density $\phi = \sum_{(i,j)} \int_0^{l_{ij}} s_{ij}(l) dl / \pi R^2$, we obtain:

$U = \frac{\pi}{2} E_0 \phi (\delta R)^2$. On the other hand, the actual potential energy U^* is equal to half the work done by the external forces [Love (1927)]: $U^* = \frac{1}{2} \delta P 2\pi R \delta R = 2\pi \kappa^{(2D)} (\delta R)^2$. Comparison of the expressions of U and U^* finally leads to an upper-bound for the bulk modulus:

$$\kappa^{(2D)} \leq \frac{E_0 \phi}{4}. \quad (13)$$

This bound is identical to the HS upper bound 2. A similar study for 3D open-cell structures leads to the following bound for the bulk modulus $\kappa^{(3D)}$ [Durand (2005)]:

$$\kappa^{(3D)} \leq \frac{E_0 \phi}{9}. \quad (14)$$

It is worth noticing this bound is tighter than the HS upper-bound value 4, giving a sharpest estimation of the actual bulk modulus value.

Criteria for maximal bulk modulus. We now show that the bulk modulus equals the upper-bound value *if and only if* the three conditions a), b), c) are simultaneously satisfied. The demonstration is straightforward: according to the principle of minimal potential energy, the inequality 13 becomes a strict equality if and only if the trial displacement field $\mathbf{u}(\mathbf{r}) = -\frac{\delta R}{R} \mathbf{r}$ is the actual displacement field satisfying the equations of mechanical equilibrium. Inspection of force and moment balances along each edge and at each junction leads to the three necessary and sufficient conditions stated above. Let us make this precise. Consider a specific edge (i, j) (see Fig. 1b); at equilibrium, the moments of forces acting on it must balance. Choosing as referencing point for the moments the node i , and denoting $\mathbf{r}_{iM} = \mathbf{r}_M - \mathbf{r}_i$, where \mathbf{r}_i and \mathbf{r}_M are

the respective position vectors of node i and of any point M belonging to the edge, we obtain: $\mathbf{r}_{iM} \times \mathbf{F}_{ij}(l) = E_0 s_{ij}(l) \frac{\delta R}{R} \mathbf{r}_{iM} \times \mathbf{t}_{ij} = \mathbf{0}$. Thus, the tangent unit vector \mathbf{t}_{ij} must be parallel to the position vector \mathbf{r}_{iM} for any point M belonging to the edge, leading to condition a). The forces acting on any piece Δl of the straight edge (i, j) must balance as well: $E_0 \frac{\delta R}{R} s_{ij}(l) = E_0 \frac{\delta R}{R} s_{ij}(l + \Delta l)$ what immediately leads to condition b). Finally, mechanical equilibrium at every junction i is satisfied if: $\sum_j \mathbf{F}_{ij} = \mathbf{0}$, with $\mathbf{F}_{ij} = -E_0 s_{ij} \frac{\delta R}{R} \mathbf{e}_{ij}$, leading to condition c). The moment balance at every junction is automatically satisfied when conditions a), b), c) are fulfilled, since the force acting on each straight edge is then axially oriented. It can also be checked that the geometrical constraint on angles between adjoining edges is satisfied [Durand (2005)]. Besides, we must point out that the upper bound and the criteria for maximal bulk modulus can be applied to the specific case of spring networks, just by replacing the quantity $E_0 s_{ij}/l_{ij}$ for each edge (i, j) by the spring constant k_{ij} of the corresponding spring [Durand (2005)].

4 Conclusions

The upper bounds established in this paper are optimal bounds, meaning that there exist cellular materials with maximal average conductivity and bulk modulus: those which satisfy the necessary and sufficient conditions a), b), c). Actually, since these conditions are independent of the connectivity of the junctions, there is an infinity of optimal structures. Various examples can be found in literature: we can cite the square, hexagonal, triangular, kagomé cells [Torquato *et al.* (1998); Hyun-Torquato (2002)] as 2D structures, and the cubic [Gibson-Ashby (1997)] and Kelvin cells [Warren-Kraynik (1988); Zhu *et al.* (1997)] as 3D structures.

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